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STRUCTURE FILE UPDATES:   17 JUL 2005  HIGHEST RN 855596-49-5
DICTIONARY FILE UPDATES:  17 JUL 2005  HIGHEST RN 855596-49-5

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*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
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Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
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=> file caplus
FILE 'CAPLUS' ENTERED AT 15:12:42 ON 18 JUL 2005
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FILE COVERS 1907 - 18 Jul 2005  VOL 143 ISS 4
FILE LAST UPDATED: 17 Jul 2005  (20050717/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
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substance identification.

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=> d stat que L13
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H 38
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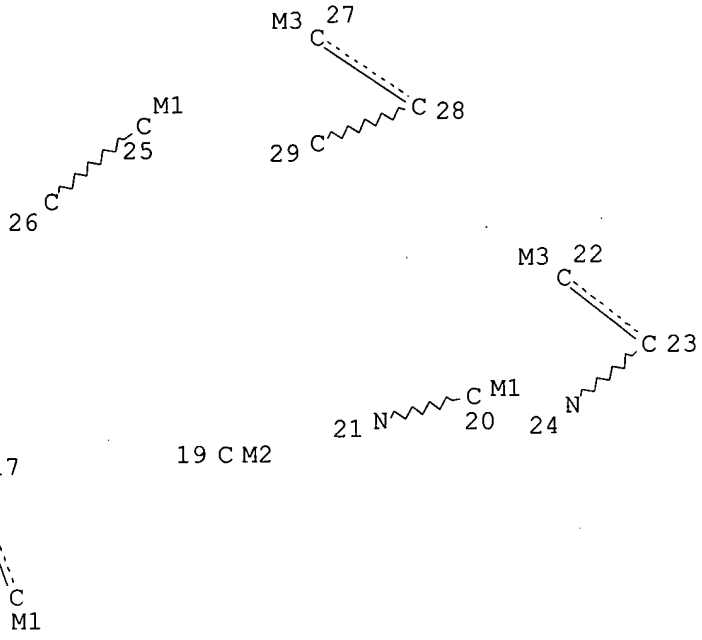

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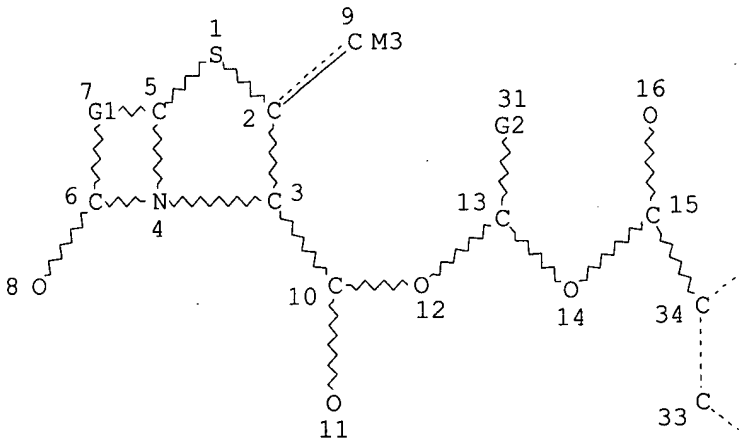

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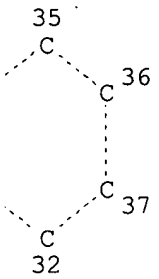

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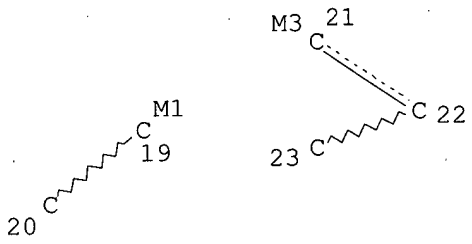

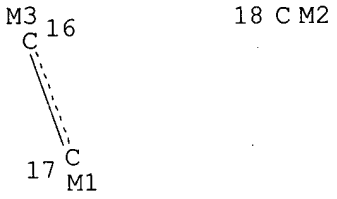

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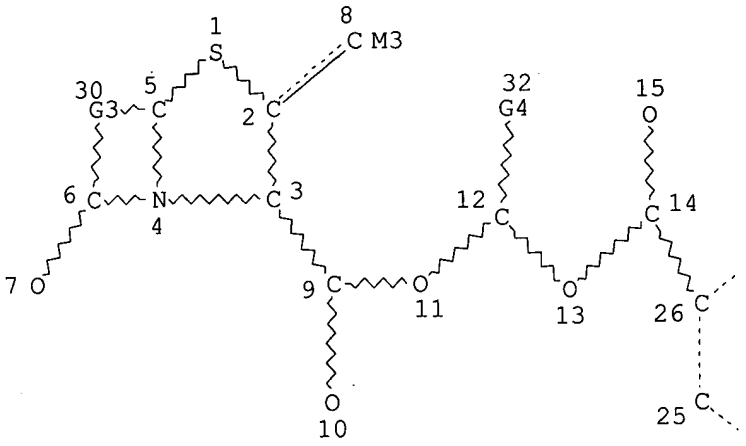

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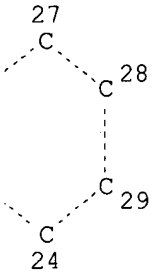

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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  33

STEREO ATTRIBUTES: NONE
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=> d ibib abs hitstr L13 1-4

L13  ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2004:182891  CAPLUS
DOCUMENT NUMBER:          140:217438
TITLE:                    Preparation of hydroxymethylpenicillanic acid sulfones
                          as β-lactamase inhibitor prodrugs
INVENTOR(S):              Marfat, Anthony; McLeod, Dale Gordon
PATENT ASSIGNEE(S):       Pfizer Products Inc., USA
SOURCE:                   PCT Int. Appl., 83 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     WO 2004018484         A1    20040304    WO 2003-IB3582          20030811
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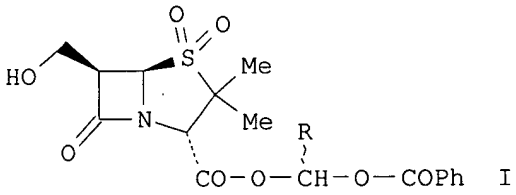


I

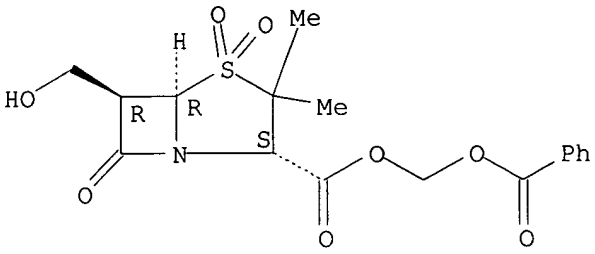
AB Prodrugs of 6β-hydroxymethylpenicillanic acid sulfone of formula I [R = H, Me] and solvates thereof, are prepared Also disclosed are pharmaceutical compns. comprising a prodrug of the present invention, or a solvate thereof, an optional β-lactam antibiotic and at least one pharmaceutically acceptable carrier. Further disclosed is a method for increasing the therapeutic effectiveness of a β-lactam antibiotic in a mammal by administering an effective amount of a β-lactam antibiotic and an effectiveness-increasing amount of a prodrug of the present invention, or a solvate thereof. Addnl. disclosed is a method for treating a bacterial infection in a mammal by administering a therapeutically effective amount of a pharmaceutical composition of the present invention to a mammal in need thereof. Thus, a combination of amoxicillin and prodrug I (R = (R)-Me) was effective against S. pneumoniae in gerbil otitis media model.

IT **666174-85-2P 666174-86-3P 666174-87-4P 666174-88-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hydroxymethylpenicillanic acid sulfones as β-lactamase inhibitor prodrugs)

RN 666174-85-2 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-(hydroxymethyl)-3,3-dimethyl-7-oxo-, (benzoyloxy)methyl ester, 4,4-dioxide, (2S,5R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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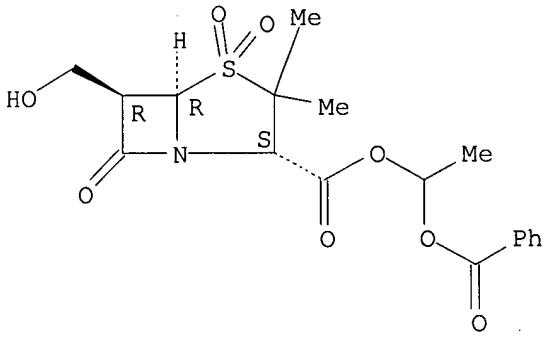
Absolute stereochemistry.



RN 666174-87-4 CAPLUS
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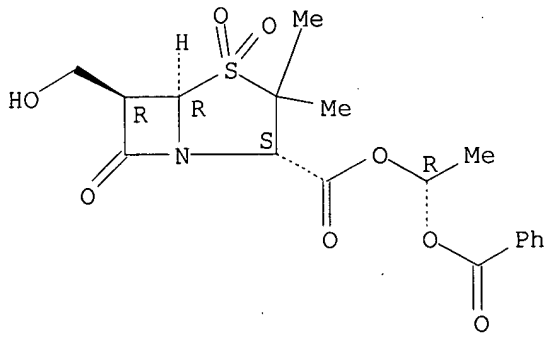
Absolute stereochemistry. Rotation (+).



RN 666174-88-5 CAPLUS
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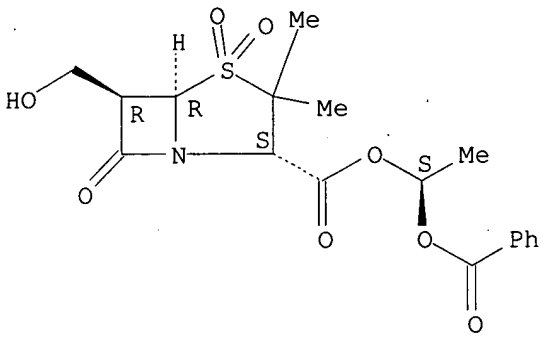
Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:591536 CAPLUS
DOCUMENT NUMBER: 101:191536
TITLE: 1,1-Alkanediol dicarboxylate-linked antibacterial agents
INVENTOR(S): Jasys, Vytautas J.; Kellogg, Michael S.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S., 39 pp. Cont.-in-part of U.S. Ser. No. 334,022, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4457924	A	19840703	US 1982-429915	19820930
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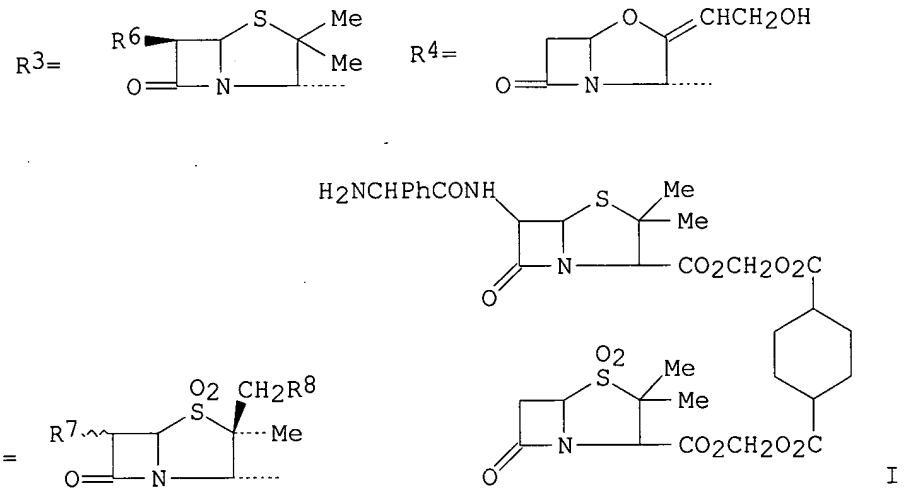

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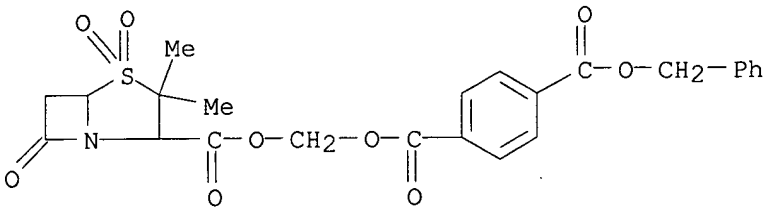
AB RCO2CHR1O2CXO2C(CHR1O2C)nR2 [X = C1-12 alkylene, alkylidene (un)substituted by Ph or CO2H, cycloalkylene, phenylene, naphthalenediyl, furandiyl, thiophendiyl, pyridinediyl, pyrazinediyl; R = R3-R5; R1 = H, alkyl; R2 = R3-R5, H, alkyl, CH2Ph, CHR1Cl, CHR1I, NBu4; R6 = NH2, 2,6-(MeO)2C6H3CONH, PhOCH2CONH, 4-R9C6H4CHR10CONH; R7 = H, CH2OH, CH2NH2, CHMeNH2; R8 = H, Cl, OAc; R9 = H, OH, acyloxy, alkoxycarbonyloxy, (un)substituted BzO; R10 = H, (un)protected NH2, N3] were prepared Thus, I was prepared from Na penicillanate 1,1-dioxide, ampicillin, K benzyl trans-1,4-cyclohexanedicarboxylate, ClCH2I, and ClCH2Br in 10 steps.

IT **87343-43-9P 87343-50-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)
RN 87343-43-9 CAPLUS
CN 1,4-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)



RN 87343-50-8 CAPLUS
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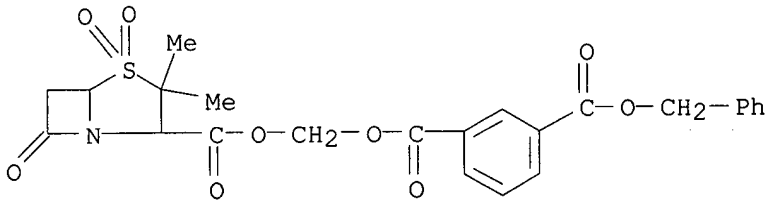
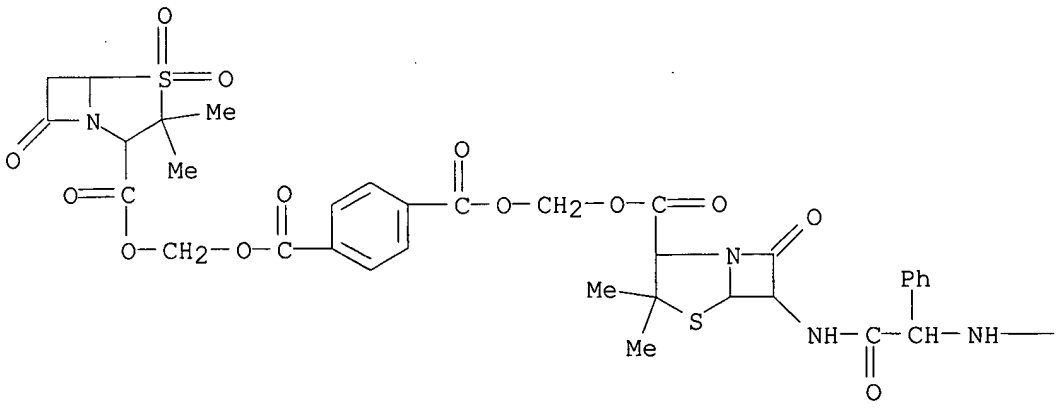


IT **87352-91-8P 87352-93-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 87352-91-8 CAPLUS
CN 1,4-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl [[[6-[[[(3-methoxy-1-methyl-3-oxo-1-propenyl)amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl ester, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)

PAGE 1-A



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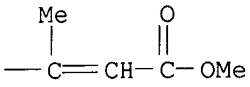

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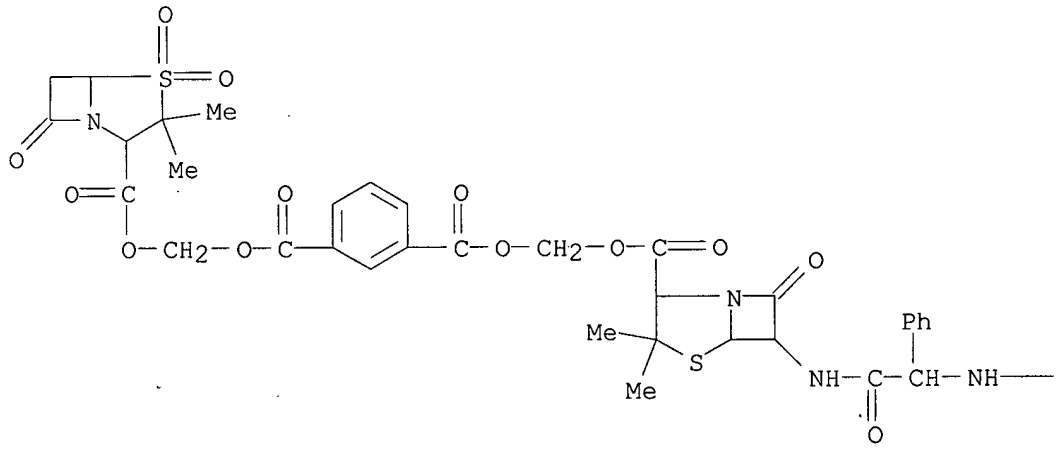
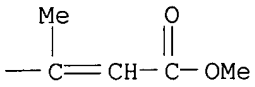
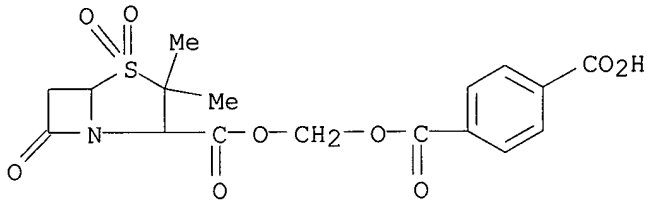
CN 1,3-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl [[[6-[[[(3-methoxy-1-methyl-3-oxo-1-propenyl)amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl ester, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)

PAGE 1-A



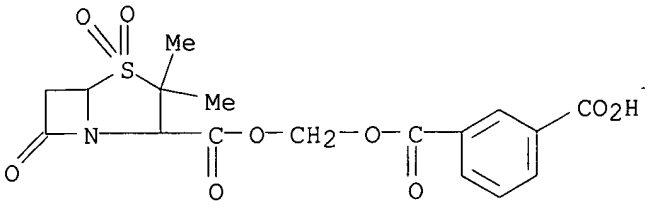


IT **87343-44-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and neutralization of)
RN 87343-44-0 CAPLUS
CN 1,4-Benzenedicarboxylic acid, mono[[[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl] ester, sodium salt, (2S-cis)- (9CI) (CA INDEX NAME)



● Na

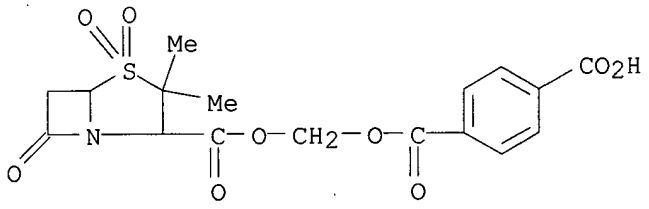
IT **87343-51-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ampicillin iodomethyl ester)
RN 87343-51-9 CAPLUS
CN 1,3-Benzenedicarboxylic acid, mono[[[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl] ester, sodium salt, (2S-cis)- (9CI) (CA INDEX NAME)



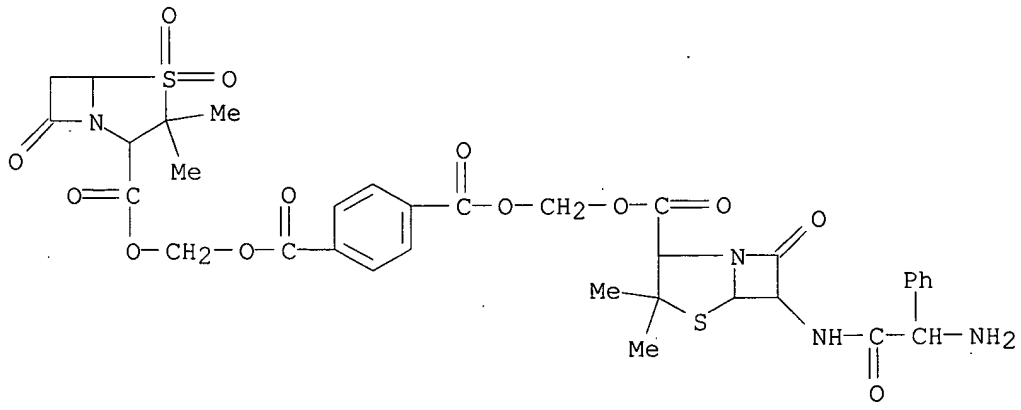
● Na

IT **87343-45-1 87352-92-9 87503-35-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetoacetate)

RN 87343-45-1 CAPLUS
CN 1,4-Benzenedicarboxylic acid, mono[[[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

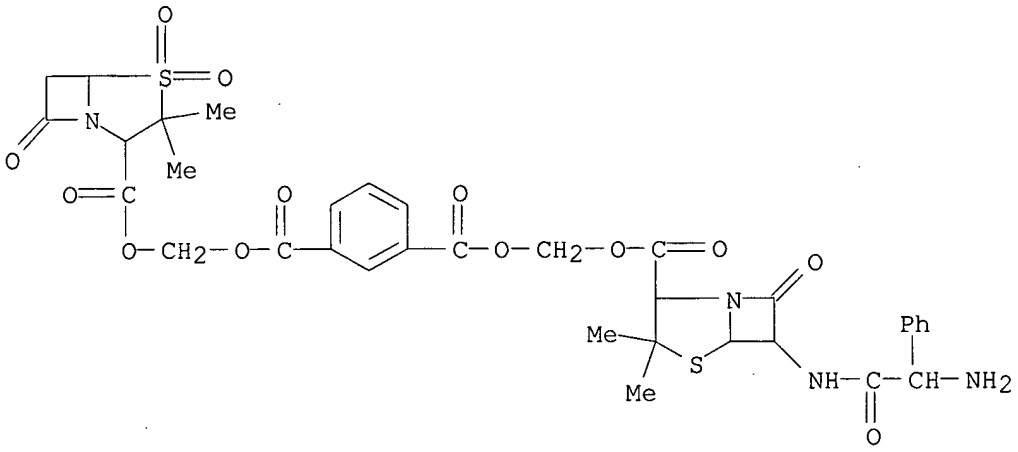


RN 87352-92-9 CAPLUS
CN 1,4-Benzenedicarboxylic acid, [[[6-[(aminophenylacetyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl ester, monohydrochloride, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)



● HCl

RN 87503-35-3 CAPLUS
CN 1,3-Benzenedicarboxylic acid, [[[6-[(aminophenylacetyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl ester, monohydrochloride, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)



● HCl

L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:6194 CAPLUS
DOCUMENT NUMBER: 100:6194
TITLE: 1,1-Alkanediol dicarboxylate linked antibacterial agents
INVENTOR(S): Jasys, Vytautas John; Kellogg, Michael Stephen
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: Eur. Pat. Appl., 124 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 83484	A1	19830713	EP 1982-306683		19821214
EP 83484	B1	19860219			
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE					
US 4457924	A	19840703	US 1982-429915		19820930
AT 18051	E	19860315	AT 1982-306683		19821214
PRIORITY APPLN. INFO.:			US 1981-334022	A	19811222
			US 1982-429915	A	19820930
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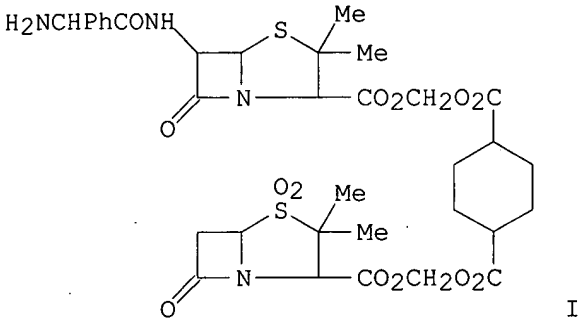


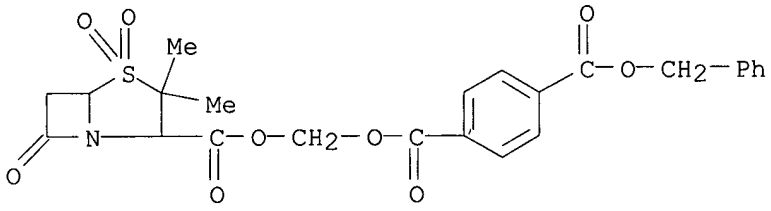
I

AB Diesters of alkanedicarboxylic acids with penicillin esters and penicillanates, penicillanate dioxides, or hydroxyethyleneoxaazabicyclohep tanecarboxylates were prepared Thus, I was obtained from Na penicillanate dioxide, ampicillin, and K benzyl trans-1,4-cyclohexanedicarboxylate, ClCH2I, and BrCH2Cl in 10 steps.

IT **87343-43-9P 87343-50-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)

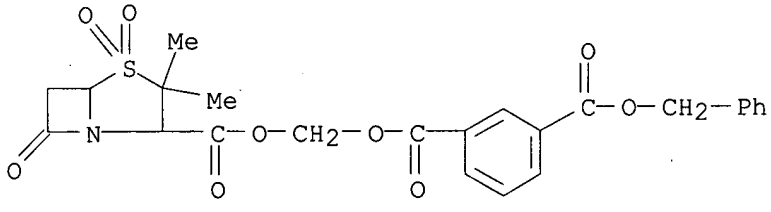
RN 87343-43-9 CAPLUS

CN 1,4-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)



RN 87343-50-8 CAPLUS

CN 1,3-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

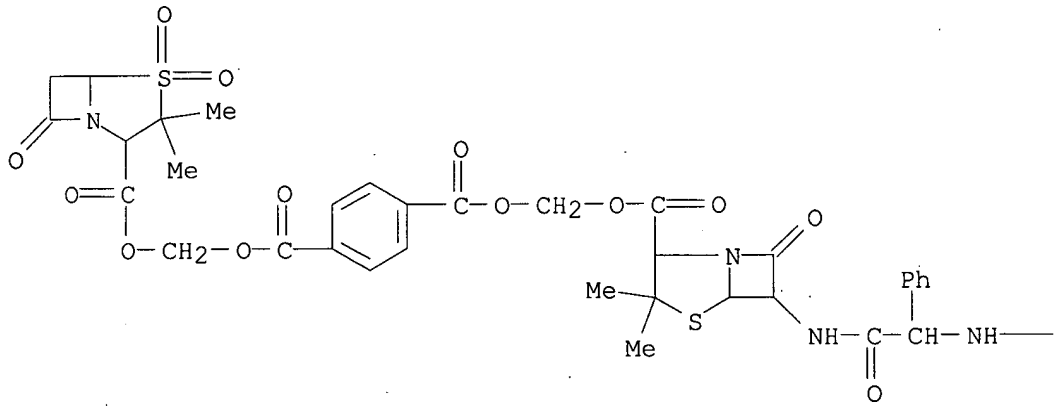


IT **87352-91-8P 87352-93-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

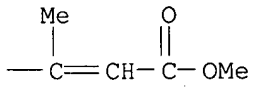
RN 87352-91-8 CAPLUS

CN 1,4-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl [[[6-[[[(3-methoxy-1-methyl-3-oxo-1-propenyl)amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl ester, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)

PAGE 1-A



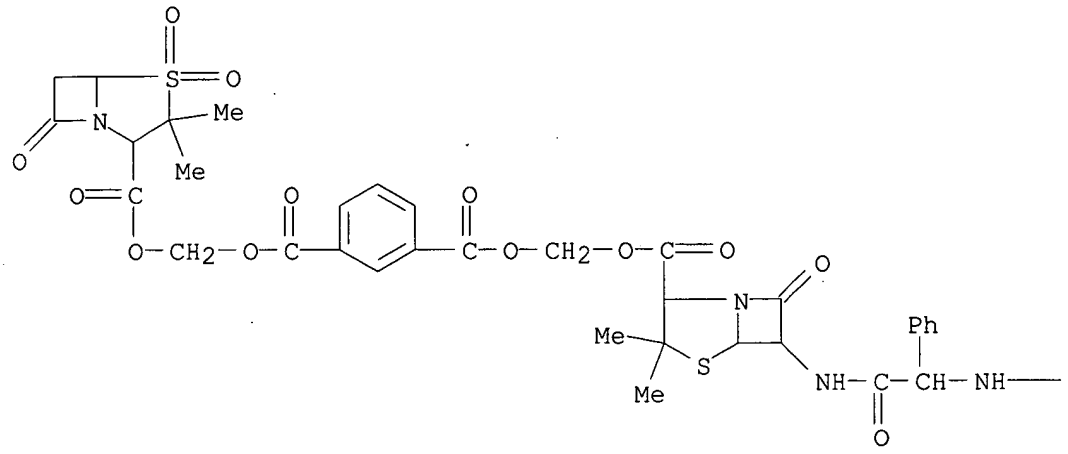
PAGE 1-B



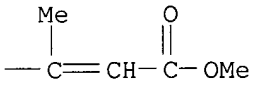
RN 87352-93-0 CAPLUS

CN 1,3-Benzenedicarboxylic acid, [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl [[[6-[[[(3-methoxy-1-methyl-3-oxo-1-propenyl)amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl ester, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)

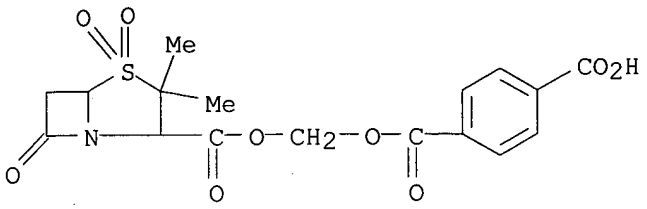
PAGE 1-A



PAGE 1-B

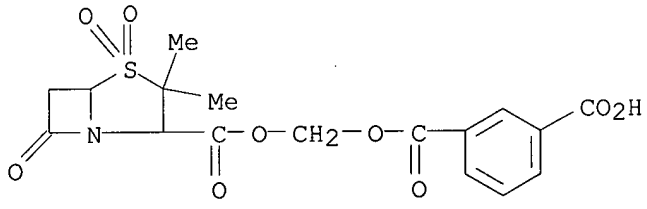


IT **87343-44-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and neutralization of)
RN 87343-44-0 CAPLUS
CN 1,4-Benzenedicarboxylic acid, mono[[[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl] ester, sodium salt, (2S-cis)- (9CI) (CA INDEX NAME)



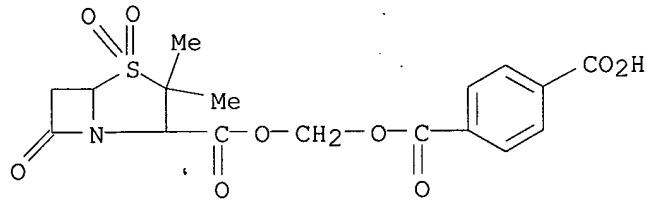
● Na

IT **87343-51-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ampicillin iodomethyl ester)
RN 87343-51-9 CAPLUS
CN 1,3-Benzenedicarboxylic acid, mono[[[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl] ester, sodium salt, (2S-cis)- (9CI) (CA INDEX NAME)



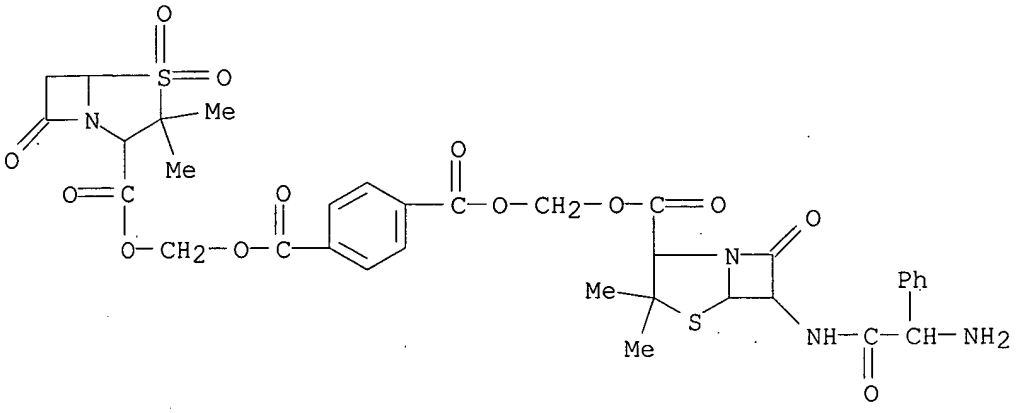
● Na

IT **87343-45-1P 87352-92-9P 87503-35-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87343-45-1 CAPLUS
CN 1,4-Benzenedicarboxylic acid, mono[[[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)



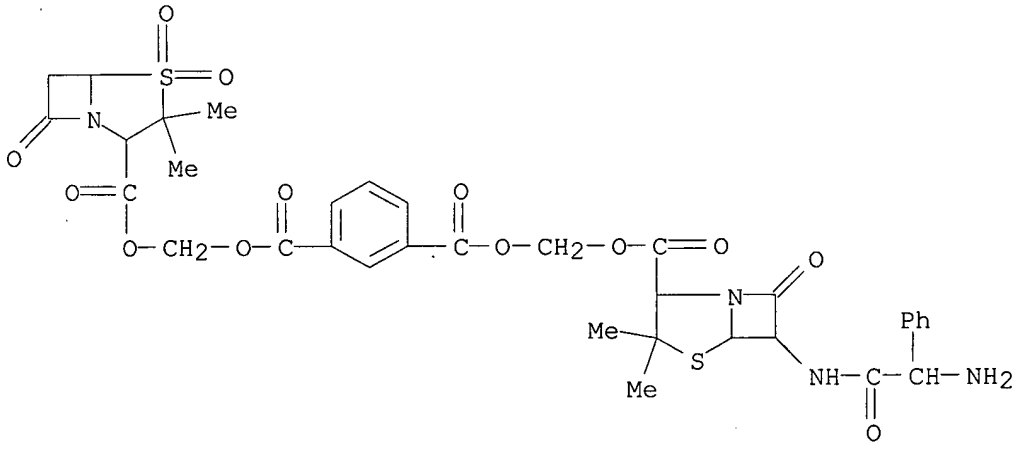
RN 87352-92-9 CAPLUS
CN 1,4-Benzenedicarboxylic acid, [[[6-[(aminophenylacetyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-

yl)carbonyl]oxy]methyl ester, monohydrochloride, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)



● HCl

RN 87503-35-3 CAPLUS
CN 1,3-Benzenedicarboxylic acid, [[[6-[(aminophenylacetyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl]carbonyl]oxy]methyl [[(3,3-dimethyl-4,4-dioxido-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl)carbonyl]oxy]methyl ester, monohydrochloride, [2S-[2α(2R*,5S*),5α,6β(S*)]]- (9CI) (CA INDEX NAME)



● HCl

L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:600528 CAPLUS
DOCUMENT NUMBER: 99:200528

TITLE: Treating resistant bacteria including anaerobes
INVENTOR(S): Gordon, Maxwell; Pachter, I. Jacob
PATENT ASSIGNEE(S): Bristol-Myers Co. , USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4406887	A	19830927	US 1981-310346	19811013
JP 60061528	A2	19850409	JP 1983-165347	19830909
EP 134302	A1	19850320	EP 1983-109144	19830915
EP 134302	B1	19870616		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
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PRIORITY APPLN. INFO.:			US 1981-310346	19811013
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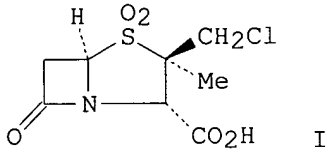

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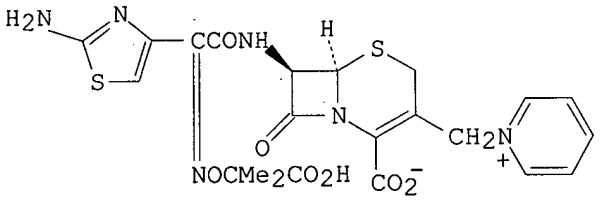


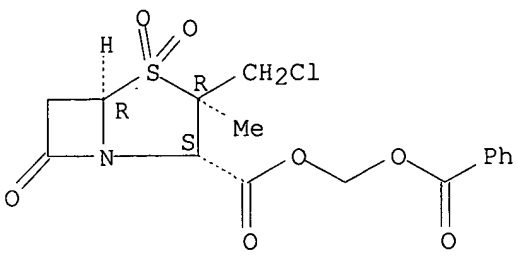
II

AB A synergistic combination of BL-P2013 (I) [79634-05-2] or its salts, as β-lactamase inhibitors, and ceftazidime (II) [72558-82-8] is used to treat bacteroides infection, especially by parenteral administration. Marked synergism was found for I and II against a number of bacteria compared with I or II alone. An injection composition was prepared containing II 500, I K salt [79634-05-2] 500 and Na2CO3 47 mg.

IT **87877-18-7**
RL: BIOL (Biological study)
(bactericidal compns. containing synergistic combination of ceftazidime with)

RN 87877-18-7 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3-(chloromethyl)-3-methyl-7-oxo-, (benzoyloxy)methyl ester, 4,4-dioxide, [2S-(2α,3β,5α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


H
O
O
S
R
CH2Cl
R
Me
S
N
O
O
O
O
Ph
O

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=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 15:15:59 ON 18 JUL 2005
COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON APRIL 21, 2005

FILE COVERS 1771 TO 2004.
*** FILE CONTAINS  9,218,366 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                 *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE    *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE           *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                         *
* FOR PRICE INFORMATION SEE HELP COST                                 *
**********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
  COMPOUND AT A GLANCE.

=> s L8 full sss
FULL SEARCH INITIATED 15:16:09 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED -    570 TO ITERATE

100.0% PROCESSED      570 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.16

L14           0 SEA SSS FUL L8
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FULL HISTORY


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L1                STRUCTURE UPLOADED
L2              6 SEA SSS SAM L1
                  D SCA

     FILE 'STNGUIDE' ENTERED AT 14:29:03 ON 18 JUL 2005

     FILE 'REGISTRY' ENTERED AT 14:30:02 ON 18 JUL 2005
L3                STRUCTURE UPLOADED
L4              5 SEA SSS SAM L3
                  D SCA

     FILE 'CAPLUS' ENTERED AT 14:31:38 ON 18 JUL 2005
L5              5 SEA ABB=ON  PLU=ON  L4

     FILE 'REGISTRY' ENTERED AT 14:42:20 ON 18 JUL 2005
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                  D L4
                  D L3
L6             76 SEA SSS FUL L3

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L7             21 SEA ABB=ON  PLU=ON  L6
L8                STRUCTURE UPLOADED
                  S L8

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L9              1 SEA SSS SAM L8

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L12            17 SEA SUB=L6 SSS FUL L8

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L16 0 SEA ABB=ON PLU=ON L15 AND L13

FILE 'REGISTRY' ENTERED AT 15:26:11 ON 18 JUL 2005

FILE 'CAPLUS' ENTERED AT 15:28:30 ON 18 JUL 2005

FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 JUL 2005 HIGHEST RN 855596-49-5
DICTIONARY FILE UPDATES: 17 JUL 2005 HIGHEST RN 855596-49-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jul 15, 2005 (20050715/UP).

FILE CAPLUS

FILE COVERS 1907 - 18 Jul 2005 VOL 143 ISS 4
FILE LAST UPDATED: 17 Jul 2005 (20050717/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON APRIL 21, 2005

FILE COVERS 1771 TO 2004.
FILE CONTAINS 9,218,366 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW

* **PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**
* **NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**